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Curvature effects in carbon nanofibers[1] MINA YOON, JANE HOWE, ZHENYU ZHANG[2], Oak Ridge National Laboratory — We apply *ab initio* density density functional formalism and also use empirical van der Waals potential to study equilibrium interlayer spacings in multi-wall carbon nanotubes and carbon nanofibers. We find that the generally-accepted empirical potential describing van der Waals interaction cannot explain the experimental observation of the strong curvature effects on interlayer spacings between neighboring graphite sheets. A modified van der Waals potential including curvature effects is constructed based on the experimental observations and theoretical calculations. Furthermore, the possible mechanism on increase or decrease of interlayer spacing in carbon nanofibers will be compared with experimental data.

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